

Exploration of resonances by analytic continuation in the coupling constant

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The energy and the width of resonance states are determined by analytic continuation of bound-state energies as a function of the coupling constant (potential strength). The advantage of the method is that the existing techniques for calculation of bound states can be applied, without any modifications, to determine the position of resonances. Various numerical examples show the applicability of the method for three-body systems, including the excited states of the ${}^6\text{He}$ and ${}^6\text{Li}$.

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Although many of excited states are resonances [1] in nuclear physics, they seldom receive special attention in theoretical nuclear structure calculations. The reason is obvious: The solution of the nuclear many-body Schrödinger equation poses insurmountable difficulties even for bound states in most of the cases, and the solution for the resonances is mostly limited to two-body problems. The theoretical nuclear model calculations therefore usually treat the resonances as bound states. This approximation, however, can only be justified for very narrow resonances.

In the recent years many theoretical and experimental nuclear physicists have concentrated their research activity on unstable nuclei and the new phenomena discovered have revived the interest in resonance states as well. These nuclei are very rich in resonance states, and one of the most spectacular phenomena, the “Borromean” binding [2], is also closely related to resonances. In a Borromean system (e.g., ${}^6\text{He}$ or ${}^{11}\text{Li}$) the bound three-body system has no bound binary subsystem, but the two-body subsystems usually have a resonance. Besides these two-body resonances, one can find an example for three-body resonances and for even more complicated ones as well [2–5].

Although there are elegant and powerful techniques to find resonances as poles of the S-matrix (see e.g. [1]), these are mostly limited to simple interactions and systems. For composite nuclear systems the theoretical apparatus has been formulated for finding the energies of bound states. The easiest way is thus to use the machinery developed for bound states to gain information on resonances. There are indeed two methods widely used in nuclear and atomic physics which rely on bound state type solutions, that is, use square integrable functions. The first, the “real stabilization method” [6], solves the Schrödinger equation in a box and exploits the fact that

the energy of the resonance state remains stable against the change of box size within certain limits (the wave function is localized inside the box), while the energies of the continuum states rapidly change. The second, the complex scaling method (CSM) [7], rotates the coordinate \mathbf{r} by $e^{i\theta}\mathbf{r}$ and transforms the continuum resonance wave function to the normalizable wave function of the bound state. Both of these methods have the advantage that they use square integrable functions and therefore, after some modifications, the already existing methods of bound-state type can be applied. These two methods are known to be in an intimate connection [8]. A slight disadvantage of the real stabilization method is that in order to determine the width of a resonances one has to solve the Schrödinger equation with many different box sizes and that it becomes computer time consuming for composite systems. Moreover, the box for a many-particle system is a many-dimensional object and sometimes it is difficult to find the appropriate intervals to be changed. In practical cases the method turns out to be suitable for narrow resonances only. The complex scaling method has proved to be capable of exploring wider resonances. Its computational burden is the calculation of complex matrix elements and the solution of complex eigenvalue problem. The source of the real hardship is that the Hamiltonian is nonhermitian and the variational principle to find an energy minimum cannot be applied. A useful guiding principle for selection of the basis, therefore, has been lost and it becomes complicated to choose the appropriate trial functions.

Kukulin *et.al.* [9] suggested an even simpler method to study resonant states; the analytical continuation in the coupling constant (ACCC). Their approach is based on the intuition that the resonances can be thought as the continuation of bound states when the attraction of the interaction decreases. More precisely, they analytically continue the energy of the bound state as a function of the strength of the potential to the complex plane to reveal the width and energy of the resonance. The authors parameterize the square root of the energy by a Padé approximation as a function of the coupling constant of the potential (potential strength). The coefficients of the Padé approximation are determined by solving the Schrödinger equation for the coupling constants giving bound states. The computational demand thus amounts to solving the Schrödinger equation for bound states for several different potential strengths. The Padé approximation is chosen to approximate the square root of the

energy as a function of the coupling constant because it is more general and more powerful than other possibilities. For example, unlike a Taylor expansion it can simulate singularities of a function near the threshold.

The ACCC method was hitherto applied in a few simple test cases for two-body resonances e.g., the analytically solvable square-well potential and a macroscopic α - α system with a simple potential. The application was limited because to fix the coefficients of the Padé approximation one has to solve the bound state problem accurately. Nowadays, there are several reliable methods at hand to solve few-body problems. Before going to some really challenging applications, it is unavoidable to test the performance and to learn the limitations of the ACCC method.

The aim of this paper is to show that the ACCC is really a powerful method to study the resonances of nuclear systems. A mathematical proof is not available, and the analytical solution is available only for a few very special cases. Therefore we must rely on numerical examples for various cases. We compare the results of ACCC to other methods such as direct numerical integration (DNI) or CSM.

The ACCC assumes that the Hamiltonian of the system is written as $H(\lambda) = H_1 + \lambda H_2$, where H_2 is the attractive part of the interaction. By decreasing λ the bound state approaches the threshold (at λ_0 the energy is $E(\lambda_0) = 0$) and may become a resonance or a virtual state. In Ref. [9] it has been shown that for a two-body system, near the threshold the square root of the energy behaves as $k_l(\lambda) \sim \sqrt{\lambda - \lambda_0}$ for $l > 0$ and $k_0(\lambda) \sim (\lambda - \lambda_0)$ for S -wave. Introducing a variable $x = \sqrt{\lambda - \lambda_0}$ the analytic function k_l has two branches $k_l(x)$ and $k_l(-x)$. Due to the analyticity of these functions we can continue them into the resonance region ($\lambda < \lambda_0$) from the bound states ($\lambda > \lambda_0$). Motivated by the above functional form of k_l near the threshold, the Padé approximation of the form [9]

$$k_l(x) = i \frac{c_0 + c_1 x + c_2 x^2 + \dots + c_M x^M}{1 + d_1 x + d_2 x^2 + \dots + d_N x^N} \quad (1)$$

is used for the analytical continuation. In principle c_0 is to be zero but reserved to take care of possible errors in the determination of λ_0 . In practice c_0 is found to be much smaller than other c values.

The coefficients of the polynomials are calculated in the bound state region and therefore are real. If $\lambda < \lambda_0$ x is pure imaginary and $k_l(x)$ becomes complex. The energy and width of the resonance state is given by $E - i\Gamma/2 = k_l^2$. To determine the coefficients we are to solve the bound state problem for various coupling constants λ ($> \lambda_0$) and try to find the threshold value λ_0 ($k_l(\lambda_0) = 0$). To have a reliable approximation one has to know the accurate values of the coefficients in the Padé approximation, that is, one has to solve the bound state problem to high (typically 4 or more digits) accuracy, especially at the threshold. The stochastic variational

approach [10,11] seems to be quite appropriate for this purpose.

Since one has to solve the bound state problem many times to determine the coefficients, one may think that the ACCC would be computer time consuming for larger systems. Due to the simple linear dependence of the Hamiltonian on the coupling constant, however, one does not have to recalculate the matrix elements and the computational load is just the re-diagonalization of the Hamiltonian for different values of the coupling constant. This property makes the application especially simple.

To solve the bound state problem we use the stochastic variational method. Of course any other method may be suitable. A point to be emphasized here is that by changing the coupling constant one goes from deeply bound to weakly bound states and finally to the threshold. All these states should be accurately treated and in a variational calculation, for example, one has to choose a basis which adequately spans the configuration space.

To illustrate the method we start with a simple example. We consider a system of two-particles with mass m interacting via a two-range Gaussian potential: [12]

$$V(r) = -8\lambda \exp[-(r/2.5)^2] + 2 \exp[-(r/5)^2], \quad (2)$$

where $\hbar = c = m = 1$. This simple problem can be easily solved by DNI [13]. The trajectories of resonances of different partial waves by ACCC and by DNI are compared in Fig. 1. For simplicity we assumed $M = N$ in Eq. (1). To determine the $2M + 1$ coefficients one has to solve the bound state for $2M + 1$ different coupling constants ($\lambda_1, \dots, \lambda_{2M+1}$). Once the bound state energies are known, the coefficients of the Padé approximation can be extracted by solving a system of linear equations. Due care must be taken to avoid numerical problems. The ACCC results agree very nicely with the DNI results including the $1S$ excited resonance state.

The second example tests the effectiveness of the method for wide resonances. The wide resonances may cause serious difficulties in many cases. In this example we have used the same potential as Eq.(2) but with a lower barrier ($V_0 = 0.25$ instead of $V_0 = 2$). The results of ACCC and DNI agree very well (see Fig. 2). The results are surprisingly good considering the fact that, in the last few points where the attraction is very weak, the widths of the states are two times of their energies (one may not really call them resonances).

The third example is a three-body case. Three bosons of mass, $\hbar^2/m = 41.47$, interact via the potential

$$V(r) = -120 \exp[-r^2] + 3\lambda \exp[-(r/3)^2]. \quad (3)$$

The energy and length are in units of MeV and fm. Note that there is no two-body bound state. We compare the results of ACCC to those of CSM. This simple example is selected because the CSM might have some inaccuracy in more complex cases, and we want to address the applicability of ACCC in a clean test case. The three-body bound state problem for zero total angular momentum has been solved by the stochastic variational

method by using a Gaussian basis [11]. The trajectories of ACCC and CSM as a function of λ are shown in Fig. 3. The two methods give the same resonance position for a wide range of potential strength, justifying the suitability of ACCC. Padé approximations with $M=3, 5$ and 7 are used. By increasing the number of terms the agreement slightly improves but already $M=3$ terms give good results. Except for the threshold value, one has the freedom to choose those coupling constants for which the bound state problem is solved to determine the coefficients of the Padé approximations. The position of the resonance, of course, depends on the choice of the set of λ . We found that if the values of coupling constants used are distributed into a wide range the dependence of the resonance parameters E and Γ on the input values are relatively small. The sensitivity can be easily controlled by comparing the results starting from several adequately chosen input sets.

The resonance states of the $\alpha + N + N$ three-body model are chosen as a practical example. These resonances have been very intensively studied in the past [3,4] and the investigation is continued with great elan [2,5]. Previously, we described the bound states of the ${}^6\text{He}$ and ${}^6\text{Li}$ nuclei in an $\alpha + n + n$ and $\alpha + p + n$ -type microscopic cluster model with the stochastic variational method [11,14]. To determine the resonances of these systems by ACCC, we used the same type of bound state solutions. The model assumes an alpha cluster but uses a fully microscopic six-body wave function. The nucleons interact via the Minnesota effective interaction (sum of the Coulomb and spin-isospin dependent central and spin-orbit potentials) [15]. The strength of the attraction of the potential is controlled through the space exchange mixture parameter u . Note, that due to the simple harmonic oscillator shell model description of the alpha particle, the change of the potential parameter u does not change the energy of the α -particle and thus the three-body threshold remains the same. The wave function of the system is taken as linear combination of terms describing the $\alpha(NN)$ and $(\alpha N)N$ arrangements. The details of the model is given elsewhere [14]. To compare the results to other calculations the parameters and the model space of Ref. [5] have been adopted.

Table I compares the results of ACCC with those of CSM. The CSM is not an exact solution, and especially for complex systems, the results of CSM might have inherited some inaccuracies from the underlying gaussian expansion and numerical inaccuracies due to the complex arithmetics [5]. The results of ACCC and CSM therefore should be consistent within "error bars". Bearing in mind that both methods attempt to solve a composite system starting from a fully microscopic model, the agreement of the result can be considered to be very good. These examples show that the ACCC can be combined with a microscopic structure model. The ACCC might be applied in combination with other microscopic method like shell model or Hartree-Fock method.

In a three-body system, the form of singularity in the

coupling constant is likely to be different from that of the two-body case. The need for higher order terms in the Padé-approximation may reflect this incorrectness. The knowledge of the analytical form of the near threshold singularities would make the convergence (in the terms of Padé-expansion) faster.

In summary, we have shown through various examples that the ACCC is really a powerful method to cope with resonances of nuclear systems. The application of the ACCC method has been made possible by the recent developments in solving bound state type problems and the increase of computational power. The results of the ACCC method have been compared to those of other solutions and are found to be in good agreement.

The advantage of the ACCC over the CSM is that one does not need to calculate complex matrix elements, that one does not have to use complex arithmetics on the computer. Unlike the real stabilization method, one does not need to recalculate the Hamiltonian on different bases many times. On the other hand, to have a reliable solution by the ACCC method, one has to solve the bound state problems very accurately. This requirement may pose certain limitations in applications. The determination of resonances by the direct solution of the Faddeev-equation [16,17] is certainly superior, but the ACCC seems to be more easily applicable in the framework of microscopic models.

The results encourage the application of ACCC to study the resonance states of few-nucleon and few-cluster systems.

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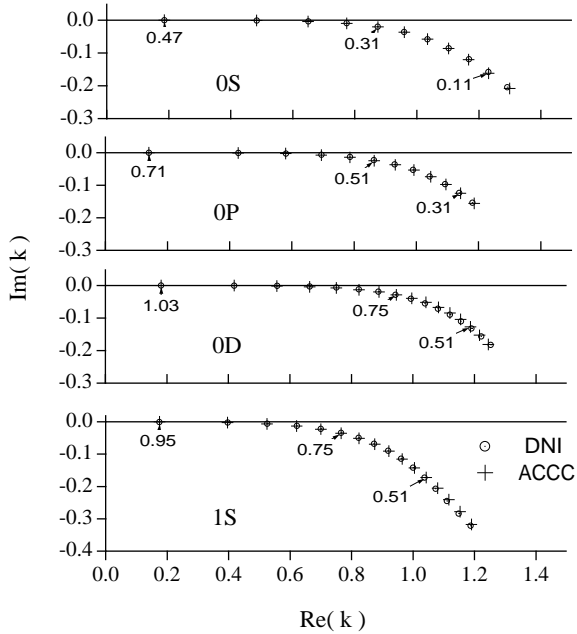


FIG. 1. The resonances for the two-range Gaussian potential of Eq.(2). The ACCC results with $M=N=5$ are compared with those of direct numerical integration (DNI). The trajectories of the resonances are plotted as a function of the coupling constant λ at intervals of $\delta\lambda = 0.04$.

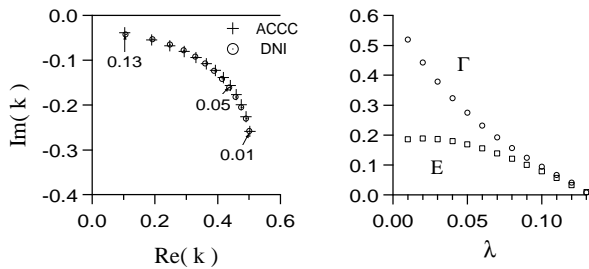


FIG. 2. The trajectories of wide S -wave resonances. The same as Fig.1 but the barrier height is reduced as described in text. The Pad6 approximation with $M=N=19$ is used. The energy and the width of the resonance are also shown as a function of λ .

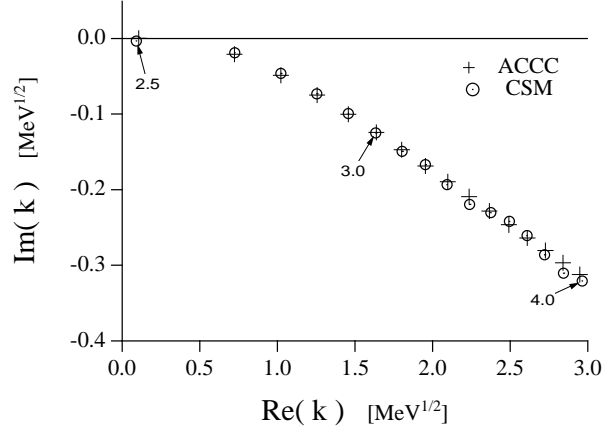


FIG. 3. The resonances of the three-boson system interacting via the potential of Eq. (3). The ACCC results with $M=N=7$ are compared with those of the complex scaling method (CSM). The trajectories of the resonances are plotted as a function of the coupling constant λ at intervals of $\delta\lambda = 0.1$.

TABLE I. Comparison of resonance energy and width between ACCC and CSM. The energy is from the three-body threshold.

${}^6\text{He}(2^+, T=1) (M, N)$	E [MeV]	Γ [MeV]
ACCC (9,9)	0.73	0.07
CSM ^{a)}	0.74	0.06
Exp ^{b)}	0.82 ± 0.025	0.133 ± 0.020
${}^6\text{Li}(0^+, T=1)$		
ACCC (9,9)	0.21	0.003
CSM ^{a)}	0.22	0.001
Exp ^{b)}	-0.137	
${}^6\text{Li}(2^+, T=1)$		
ACCC (9,9)	1.61	0.27
CSM ^{a)}	1.59	0.28
Exp ^{b)}	1.696 ± 0.015	0.54 ± 0.020

a) Ref [5], b) Ref [18]